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14. ABSTRACT This is a final report on a workshop entitled "Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials" that was held at Johns Hopkins University on September 5-6, 2013. The event consisted of 2 introductory talks, 11 plenary talks and a host of panel discussions. The talks and panel discussions were able to identify areas of opportunities that exist with respect to future research directions sponsored by the Army Research Office in the field of Solid Mechanics. Serious gaps remain in a consistent approach for integrated computational material structure modeling that is needed for					
15. SUBJECT TERMS Computational Structure Heterogeneous Material Models					
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a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 410-516-8690

Report Title

Final Report: Challenges in Integrated Computational Structure - Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials

ABSTRACT

This is a final report on a workshop entitled “Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials” that was held at Johns Hopkins University on September 5-6, 2013. The event consisted of 2 introductory talks, 11 plenary talks and a host of panel discussions. The talks and panel discussions were able to identify areas of opportunities that exist with respect to future research directions sponsored by the Army Research Office in the field of Solid Mechanics. Serious gaps remain in a consistent approach for integrated computational material-structure modeling that is needed for developing predictive capabilities of high strain-rate deformation, damage and failure in heterogeneous materials for DoD applications. The Computational Mechanics and Mechanics of Materials communities have made important strides towards advancing modeling capabilities in dynamic material behavior. However a comprehensive integrated approach, coupling novel developments and innovations in the fields of multi-scale computational mechanics and materials engineering, leading to prediction of structure-materials response and failure behavior is still missing. Development of a framework that couples multi-scale computational mechanics, materials science, and experiments for response of failure analysis under dynamical loading is seen as an important initiative that can be advanced by ARO.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received

Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

There were 11 presentations made at the workshop. They are:

- 1. J. Zheng, An Army Perspective and Expected Outcome
- 2. S. Ghosh, Challenges in Integrated Computational Structure-Material Modeling
- 3. A.M. Rajendran, Challenges and issues in modeling heterogeneous materials
- 4. M. Zikry, Microstructural Modeling of High Strain-Rate in Crystalline Metals Alloys
- 5. S. De, Jacobian-free Multiscale Methods
- 6. C. Bronkhorst, Computational/Experimental Interrogation of Dynamic Damage Nucleation in Polycrystalline Metallic Materials
- 7. K. T. Ramesh, CMEDE Summary of Activities
- 8. R. Ghanem, Uncertainty Quantification for Predictive Modeling of Materials.
- 9. M. Ebeida, Algorithms for Well-spaced Random Points for Uncertainty, Optimization, Meshing, Graphics and Robotics
- 10. R. Suter, HEDM Tracking of Microstructure Responses with Direct Comparison to Image Based Models
- 11. T. Pollock, 3D Characterization of Microstructure and Material Damage

Number of Presentations: 11.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts	
<u>Received</u>	<u>Paper</u>
TOTAL:	

Number of Manuscripts:

Books	
<u>Received</u>	<u>Book</u>
TOTAL:	
<u>Received</u>	<u>Book Chapter</u>
TOTAL:	

Patents Submitted	
Patents Awarded	
Awards	

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Somnath Ghosh	0.00	
FTE Equivalent:	0.00	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Total Number:

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Ji Yeon Hong	0.10
New Entry	0.00
FTE Equivalent:	0.10
Total Number:	2

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

The workshop entitled “Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials” was held on the campus of Johns Hopkins University on September 5-6. The event consisted of the following:

- (i) Introductory talk on Army perspectives by Dr. J. Zheng of ARL,
- (ii) Introductory talk on the gaps and needs in the development of a robust framework for integrated computational structure-material modeling of high strain-rate deformation and failure in heterogeneous materials by Prof. S. Ghosh of JHU
- (iii) Plenary session # 1 on Physics-Based Spatial and Temporal Multi-Scale Model Development with 4 talks by Dr. A.M. Rajendran of U. Miss, Dr. M. Zikry of NC State, Dr. S. De of RPI and Dr. C. Bronkhorst of LANL. This was followed by a 30 min. panel discussion.
- (iv) Plenary session # 2 on Probabilistic Modeling & Uncertainty Quantification with 2 talks by Dr. R. Ghanem of USC and Dr. M. Ebeida of SNL. This was followed by a 30 min. panel discussion.
- (v) Plenary session # 3 on Multi-Scale Data Acquisition, Characterization & Image-Based Virtual Models with 2 talks by Dr. R. Suter of CMU and Dr. T. Pollock of UCSB. This was followed by a 30 min. panel discussion.
- (vi) Plenary session # 4 on Experimental Methods for Constitutive Models, Response Functions and Failure Processes with 3 talks by Dr. G. Ravichandran of CalTech and Dr. K Ravi-Chandar of UT Austin and Dr. G. Subhash of UFL. This was followed by a 30 min. panel discussion.
- (vii) A 1 hour panel discussion summarizing the outcome of the workshop.

The talks and panel discussions were able to identify areas of opportunities that exist with respect to future research directions. In particular, serious gaps remain in a consistent approach for integrated computational material-structure modeling that is needed for developing predictive capabilities of high strain-rate deformation, damage and failure in heterogeneous materials for Army applications. All talks where possible were collected and will be available as support to this report to participants and ARO.

Overall Summary and Recommendations

Effective multi-scale modeling of dynamic response and failure of materials at high strain-rates is of considerable interest to the DoD community for design and development of novel armor and ammunitions. Over the last few decades, the Computational Mechanics and Mechanics of Materials communities have made important strides towards advancing modeling capabilities in dynamic material behavior. However, an important aspect that has not been adequately addressed is a comprehensive integrated approach, coupling novel developments and innovations in the fields of multi-scale computational mechanics and materials science and engineering, leading to prediction of structure-materials response and failure behavior. This is more than isolated developments in these fields. For example, advances in multi-scale physics-based constitutive and damage representation cannot be fully realized unless these are appropriately coupled with computational methods that can represent their effects. Physics-informed adaptivity is at the core of such evolving problems that should be coupled with the constitutive and damage response. Also, the ICMSE (integrated computational materials science and engineering) thrusts in building image-based models at different scales cannot be fully realized unless they are intricately coupled with appropriate computational tools. Thus, development of a comprehensive framework that couples multi-scale computational mechanics, materials science, and experiments for response of failure analysis under dynamical loading is seen as an important initiative that can be advanced by the Army Research Office.

Summary Conclusions

The Computational Mechanics and Mechanics of Materials communities have made great strides in advancing our ability to numerically represent the dynamic response of materials over the past generation. The conversation of this meeting was an honest discussion of our ability to represent and predict dynamic damage, failure, and fragmentation of materials for applications of interest to the U. S. Army. The discussion was broad and extremely enlightening. There are many areas which remain unsolved, however one of the most urgent is in improving the physical representation of the damage and failure process through improved mechanistic based tools. The group envisioned using lower length scale physical models to articulate dominant physical processes during dynamic loading. These tools and new physical understanding would then be brought to bear on problems of significance to the Army and for which accurate numerical representation is presently out of reach. These tools could in turn be used to enhance soldier safety and for weight reduction in armored vehicles.

- 1) The general state of ductile damage modeling within the DoD/DoE complex is presently represented largely by macro-scale engineering models which are based upon the traditional Gurson approach from 1977. These are general purpose engineering models which lack specific mechanistic information and therefore do not perform well. The model is evaluated against a suite of experimental information and the parameters are generally not physically based.
- 2) Since the physical process is poorly represented through the equations representing the material, when macroscopic softening occurs during damage evolution these equations lose hyperbolicity and therefore a unique solution is generally lost.

This can lead to numerical instability and severe mesh sensitivity. Generally non-local material models are being looked at to introduce appropriate physical length scales into the equations so that the equations remain normalized throughout the damage process.

3) Traditional Lagrangian or Eulerian codes typically used within the DoD/DoE complex are generally inadequate to representing the evolving morphology and material heterogeneity important to damage evolution. Data structures are generally not well suited to handle non-local material models and new free surfaces are generally not easily created without violation of physical laws (e.g. conservation of mass or energy). Numerical advection in ALE and Eulerian codes also damages the material state variable set during remapping of information. This is especially true for damage fields where highly localized events take place and steep gradients in material state are nearly impossible to remap properly.

4) During dynamic loading new experimental techniques must be developed to measure in-situ physical events. This is currently not possible and therefore existing dynamic experimental work must be conducted in close concert with numerical micromechanical research to articulate the dominating physics of behavior during dynamic loading. We cannot develop physically based models and move away from the present tools without direct physical information.

5) Overall this is a major challenge for the materials and mechanics community and much work remains. Very tightly coupled Theoretical/Computational/Experimental programs must be performed in order to improve our numerical representation of damage and failure of materials under dynamic loading conditions.

Overall, the topic of this workshop still remains a severely challenging one for all communities involved. As yet, the world-wide community does not possess a satisfactory way in which to predict the general damage and failure of materials under the loading conditions of interest to the Army and ARO. Much of this stems from the lack of mechanistic understanding of the complex process by which materials damage and fail. We must move beyond general purpose phenomenological approaches to modeling if we are to intelligently simulate extreme loading conditions. Solving this problem satisfactorily will require tight collaboration between, experimental, theoretical, and computational communities. In fact, it would be most beneficial if the communities begin to overlap in their work and understand each other's world.

With respect to the four identified modules, contributing to the overall objectives, the following opportunities are identified.

I. Physics-Based Spatial and Temporal Multi-Scale Model Development

(a) Physics-based constitutive and damage models at higher scales from consistent homogenization of deformation and failure mechanisms at lower scales are generally missing. These models should explicitly account for morphological characteristics, as well as evolution of different mechanisms at the lower scales. Image-based micro- and mesoscopic computational models with morphological and crystallographic details at each scale, representing dominant deformation/failure mechanisms should be developed for this task. Limits of homogenization should be identified in terms of physics-based criteria. Deterministic homogenization methods should be extended to stochastic homogenization, accounting for the distributions of heterogeneous structures at each length scale.

(b) Novel spatial and temporal multi-scale models for deformation, localization, and failure of heterogeneous materials and structures should be developed. In spatial multi-scaling, hierarchical and adaptive-concurrent multi-level models may incorporate bottom-up and top-down coupling for transcending scales. Temporal multi-scaling is necessary for bridging the time-scale gap for different mechanisms. Special time-step acceleration, temporal coarse graining schemes and asynchronous time integrators are needed to overcome this bottleneck.

(c) Advanced computational methods that can adequately account for evolution of deformation and damage variables, as well as account for evolving topology with fracture and failure should be developed. Adaptive mesh/physics refinement/enrichment is a necessary ingredient. There is need for development of novel computational methods that can overcome the limitations of lower order conventional FEM.

(d) Appropriate image-based representative volume elements (RVE's) at each scale for different properties should be determined using statistical methods of microstructural characterization and micromechanical analysis. Investigations on the validity of RVE's at each scale in the presence of localization and cracking, as well as their evolution and scale-transition are important. The need for scale-dependent RVE/SVE and associated homogenization for specific properties at a given length scale.

II. Probabilistic Modeling & Uncertainty Quantification

(a) Effective use of probabilistic mechanics, incorporating data from advanced imaging into advanced modeling capabilities through uncertainty characterization of material structure, uncertainty identification in material properties and RVE, mapping material structure uncertainty to structural performance are essential ingredients of robust modeling. These methods should also be applied for validation studies.

(b) Develop the mathematics and computational methodology to couple uncertainty quantification tools with numerical simulations to make real-time assessment of when refinement of numerical treatment is necessary. Use these tools to also assess probability of failure for a simulation rather than relying entirely on predicting rare events explicitly.

III. Multi-Scale Data Acquisition, Characterization & Image-Based Virtual Models

(a) High-fidelity 3D characterization provides information about the microstructure at multiple length scales, particularly about "outlier" features which control extreme events. A closely related effort is the development of image-based models from the microstructural data. The relation between these image-based models (both CAD based and statistical) and the microstructural

characteristics should be investigated.

(b) Begin to adapt the high-fidelity 3D characterization tools presently under development to high rate environments. The physical mechanisms a material chooses to employ under high rate loading conditions will likely be different than under less severe conditions. We must obtain more mechanistic insight experimentally at higher rates. We are relying almost entirely on numerical physics calculations for this information now.

IV. Experimental Methods for Constitutive Models, Response Functions and Failure Processes

(a) Sophisticated multi-scale experiments are needed both for discovery (mechanisms) and model calibration over a range of operating conditions at different scales. They should be able to identify underlying mechanisms and provide the models with the requisite fundamental physics, chemistry, and materials science. Experiments should provide model parameters, validate key predictions, and supplement and extend the range of validity and reliability of the models.

(b) An important part of the process of representing the damage and failure response of materials is thermodynamic consistency in representing deformation. This includes large deformation plasticity. We as yet do not have a mechanistic linkage between the energy of deformation for large deformation plasticity and the microstructural evolution. As the material is deformed at different rates, where is the energy dissipated?

Technology Transfer

The final summary recommendations of this workshop was provided to the then program manager Dr. Larry Russell.

Report on Workshop on
Challenges in Integrated Computational Structure-Material Modeling of High Strain-
Rate Deformation and Failure in Heterogeneous Materials

Held at Johns Hopkins University
September 5-6
2013

Authors

Somnath Ghosh (JHU) and Curt Bronkhorst (LANL)

The workshop entitled “*Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials*” was held on the campus of Johns Hopkins University on September 5-6. The event consisted of the following:

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Workshop on

Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials

September 5-6, 2013
3rd Floor Boardroom, Hodson Hall
Johns Hopkins University, Baltimore MD

AGENDA

Day 1: September 5

1:00-1:05 PM	S. Ghosh	<i>Welcome and Introduction</i>
1:05-1:15 PM	James Zheng	<i>An Army Perspective and Expected Outcome</i>
1:15-1:40 PM	S. Ghosh	<i>Challenges in Integrated Computational Structure-Material Modeling</i>

Plenary Session #1: Physics-Based Spatial and Temporal Multi-Scale Model Development

1:40-2:05 PM	A.M. Rajendran, U Miss.	<i>Challenges and issues in modeling heterogeneous materials</i>
2:05-2:30 PM	M. Zikry, NC State	<i>Microstructural Modeling of High Strain-Rate in Crystalline Metals Alloys</i>
2:30-2:55 PM	S. De, RPI	<i>Jacobian-free Multiscale Methods</i>
2:55-3:20 PM	C. Bronkhorst, LANL	<i>Computational/Experimental Interrogation of Dynamic Damage Nucleation in Polycrystalline Metallic Materials</i>
3:20-3:50 PM	Plenary Session 1 Summary & Discussions, Moderator: J. El-Awady	

3:50-4:10 PM Coffee Break

4:10-4:40 PM	K. T. Ramesh	<i>CMEDE Summary of Activities</i>
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Plenary Session #2: Probabilistic Modeling & Uncertainty Quantification

4:40-5:05 PM	R. Ghanem, USC	<i>Uncertainty Quantification for Predictive Modeling of Materials.</i>
5:05-5:30 PM	M. Ebeida, Sandia	<i>Algorithms for Well-spaced Random Points for Uncertainty, Optimization, Meshing, Graphics and Robotics</i>
5:30-6:00 PM:	Plenary Session 2 Summary & Discussions Moderator: J. Guest	

6:30 PM Dinner at Gertrude's

Day 2, September 6

Plenary Session #3: Multi-Scale Data Acquisition, Characterization & Image-Based Virtual Models

9:00-9:25 AM	R. Suter, CMU	<i>HEDM Tracking of Microstructure Responses with Direct Comparison to Image Based Models</i>
9:25-9:50 AM	T. Pollock, UCSB	<i>3D Characterization of Microstructure and Material Damage</i>
9:50-10:20 AM	Plenary Session Summary 3 & Discussions Moderator: B. Schuster/A. Lewis	

10:20-10:45 AM Coffee Break

Plenary Session #4: Experimental Methods for Constitutive Models, Response Functions and Failure Processes

10:45-11:10 AM	G. Ravichandran, CalTech	<i>Multi-scale Experiments for Characterizing High-strain Rate Response of Metals</i>
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11:10-11:35 AM	K. Ravi-Chandar, UT Austin	<i>Challenges in the Modeling of Ductile Deformation and Failure – the need for multiscale experiments</i>
11:35-12:00 PM	G. Subhash, UFL	<i>Properties and Performance - Is There a Disconnect in Armor Ceramics? (Embracing Mechanism-Based Design over Property-Based Design)</i>
12:00-12:30 PM	Plenary Session Summary 4 & Discussions, Moderator K. Hemker	

12:30-1:30 PM	Lunch	in 3rd floor lobby
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Panel Discussion:

1:30-3:00 PM	General Discussion and Summary
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Adjourn



Challenges in Integrated Computational Structure-Material Modeling of High Strain-Rate Deformation and Failure in Heterogeneous Materials



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Departments of Civil Engineering & Mechanical Engineering

Johns Hopkins University

Acknowledgements

Army Research Office

ARO-Sponsored Workshop

September 5-6, 2013

Johns Hopkins University, Baltimore MD

Candidate Applications of Interest



Light armored vehicles
under mine blast &
improvised explosive
device



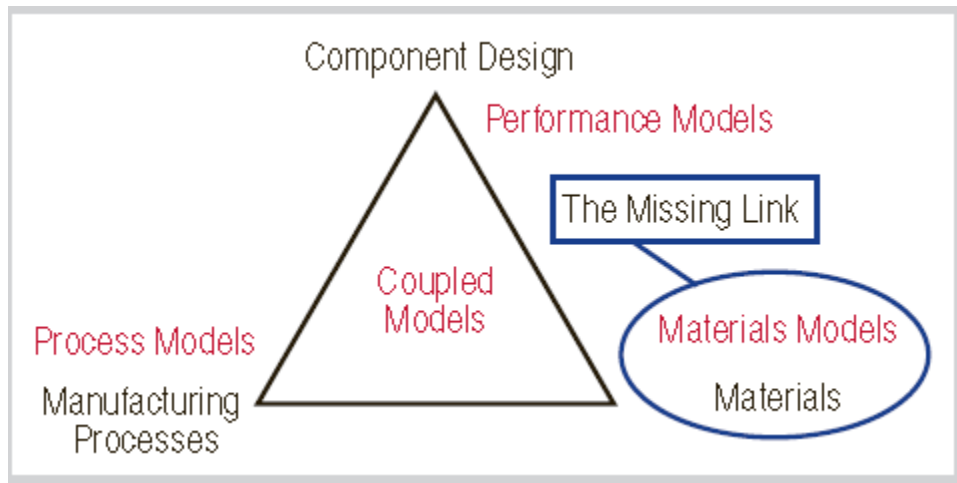
High-explosive projectile
impacting a wing section



Guided air to surface
weapon with a penetrator
and blast fragmentation
warhead.

- High demands on army applications, e.g. weapon systems, ammunition, ground structures and vehicles are challenging operational limits of conventional materials like metals, ceramics, composites.
- Design under severe thermo-mechanical conditions requires advanced methods of analysis/simulation for comprehensive understanding of structure-material behavior.

Integrated Computational Materials Science & Engineering (ICMSE) Paradigm

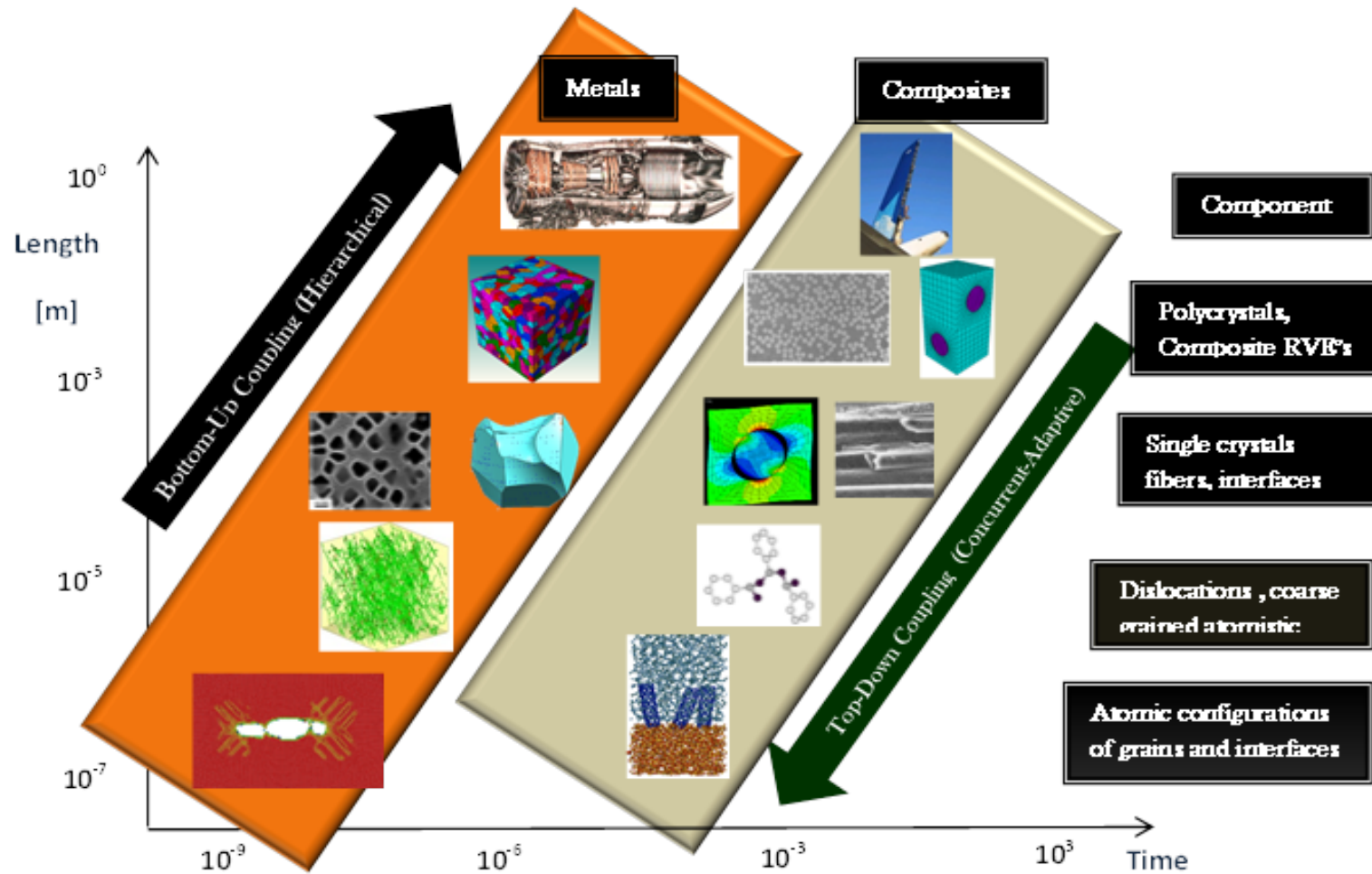


***Integrated
Computational
Materials-Structures
Engineering?***

ICMSE philosophy “*entails integration of information across **length and time scales** for all relevant materials phenomena and enables concurrent analysis of manufacturing, design, and materials within a holistic system*”

J. Allison, D. Backman, and L. Christodoulou, "Integrated Computational Materials Engineering: A new paradigm for the global materials profession," JOM, pp. 25-27, November 2006.

Multiple- Scales in Heterogeneous Materials and Structures



Multiple spatial and temporal scales for metallic and composite materials.

Various Modules Contributing to the Overall Goals

Physics-Based Spatial and Temporal Multi-Scale Model Development

- Adaptive, concurrent, multi-level models
- High-Strain-rate, Dynamic effects, Shock waves
- Microcracking, fragmentation, failure
- Lagrangian and Hydrocodes

Multi-Scale Data Acquisition, Characterization & Image-Based Virtual Models

- DB-FIB-SEM EBSD
- X-ray/ Synchrotron CT
- Characterizing/reconstructing virtual 3D microstructures

Experimental Methods for Constitutive Model and Failure Processes

- High strain rate-high pressure experiments
- Plate impact
- Laser loading microtomography

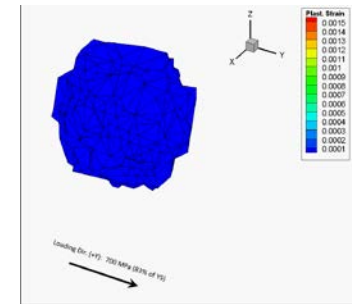
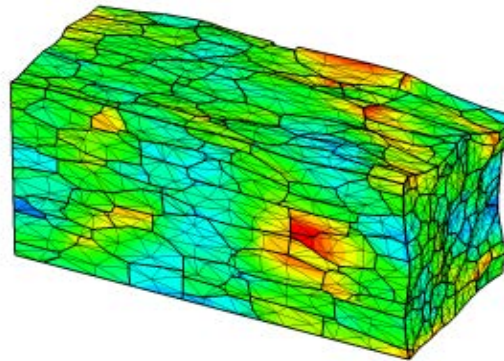
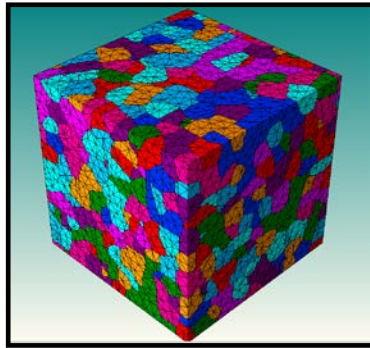
Probabilistic Modeling & Uncertainty Quantification

- Uncertainties in experimental data and models
- Uncertainty propagation analysis
- Stochastic models in homogenization

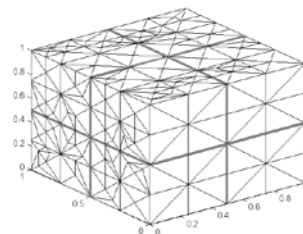
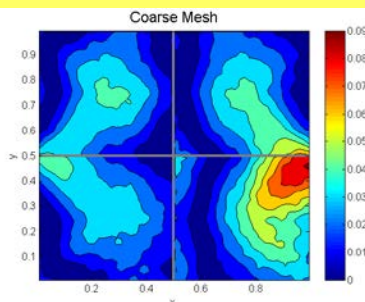


I. Physics-Based Spatial and Temporal Multi-Scale Model Development

- **Methods of image-based micro- and mesoscopic computational models with morphological and crystallographic details at each scale, representing dominant deformation/failure mechanisms**

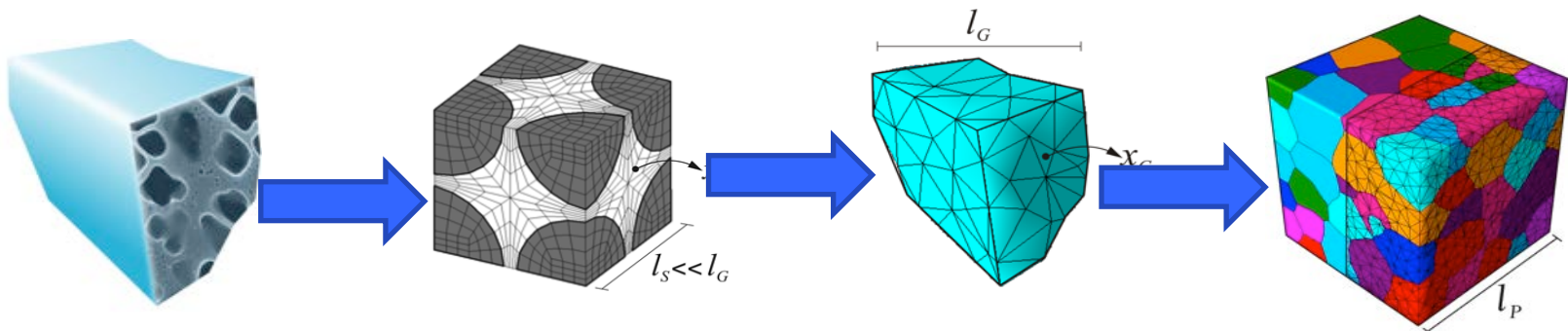


- **Shortcomings of commonly used computational methods at different scales.**
- **Alternative methods to conventional FEM, e.g. mesh-free methods, generalized FEM, or discrete approaches such as Phase-Field modeling**
- **Error indicators and adaptive methods.**



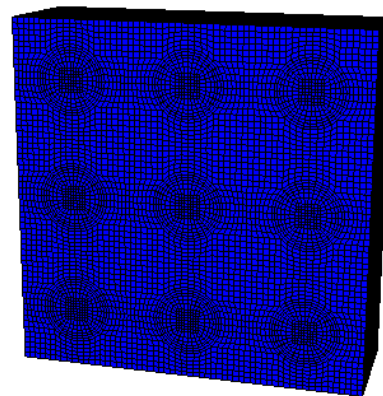
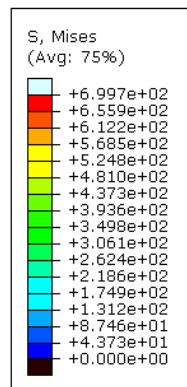
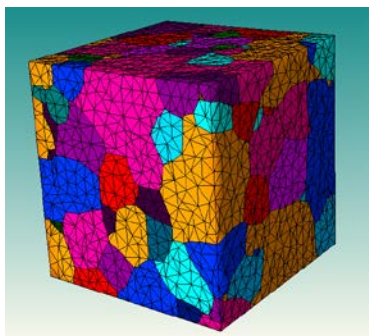
Physics-Based Spatial and Temporal Multi-Scale Model Development

- Novel spatial and temporal multi-scale models for deformation, localization, and failure of materials and structures
- Hierarchical vs. adaptive-concurrent multi-scale models incorporating bottom-up and top-down coupling
- Homogenized model representation, parameter identification and evolution laws at higher length scales from lower length scale phenomena; Reduced-order /Coarse-grained models



Physics-Based Spatial and Temporal Multi-Scale Model Development

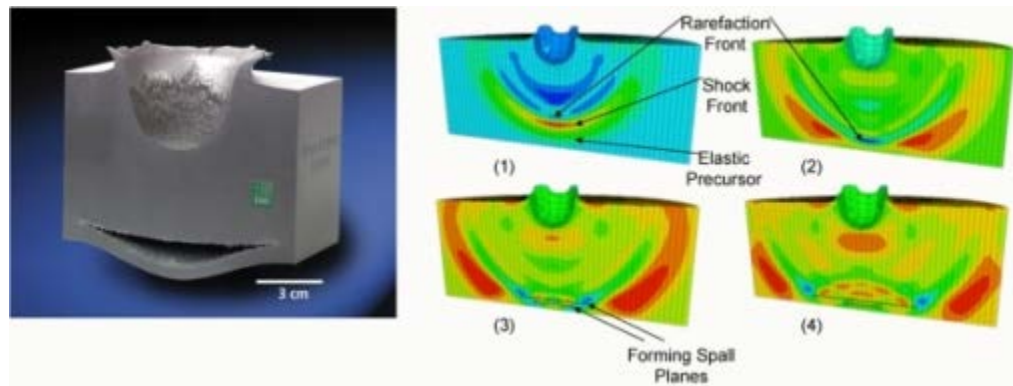
- Representative Volume Elements in Homogenization: *Image based microstructures: “exact” vs. “statistically equivalent”*.
- *RVE vs. M(microstructural) VE, P(properties) VE*
- RVE's for different properties, e.g. stiffness, strength, ductility?



- Consideration of boundary conditions in the determination of RVE (dynamic conditions, shock waves).
- Relation between morphology and response: *For nonlinearities and evolving microstructures. When does RVE size evolve?*

Physics-Based Spatial and Temporal Multi-Scale Model Development

- Modeling Instability, Localization and Failure



- Adaptive top-down multi-scaling (Concurrent models) for transcending scales.
- Higher order nonlocal models (gradient models)
- Extreme value representation: *Are higher statistical moments of relevant morphological parameters sufficient?*

Physics-Based Spatial and Temporal Multi-Scale Model Development

- Time-scale Acceleration at Discrete and Continuum Scales
- Time scales in atomistic simulations (MD) do not reach experimental time scales. *Extrapolation not valid especially in the presence of new mechanisms evolving with time*
- Methods to incorporate lower strain rates and longer time scales at lower length scales. *Hyperdynamics; Parallel Replica Dynamics*
- Multi-time scaling for multi-physics phenomena governed by different frequencies. *Special time-step acceleration, temporal coarse graining schemes and asynchronous time integrators*

Physics-Based Spatial and Temporal Multi-Scale Model Development

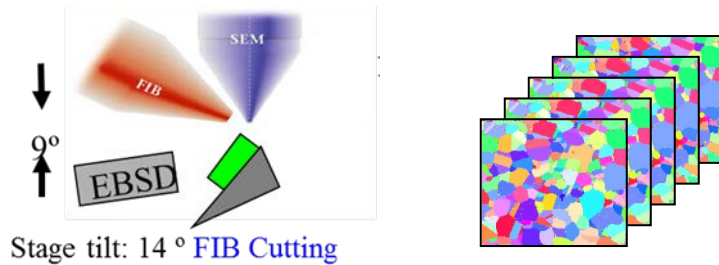
- **Modeling at Discrete Scales**
- Electronic structure by Quantum Mechanics and Density functional theory
- Thermodynamical properties, (pressure, temperature distributions) by applying statistical mechanics to reach orders of μm or nsec.
- Atomic level interpretation of deformation and mechanisms (MD)
- Discrete dislocation dynamics



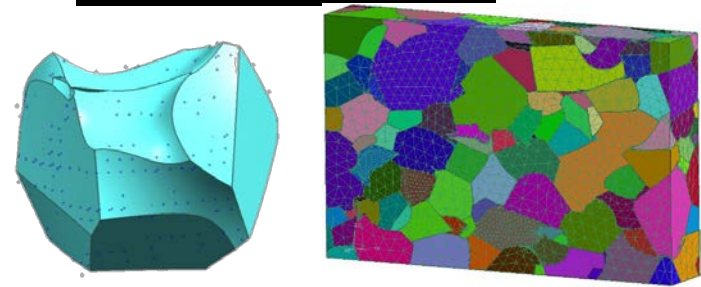
II. Multi-Scale Data Acquisition, Characterization & Image-Based Virtual Models

- Methods of constructing virtual models from advanced microstructural characterization.

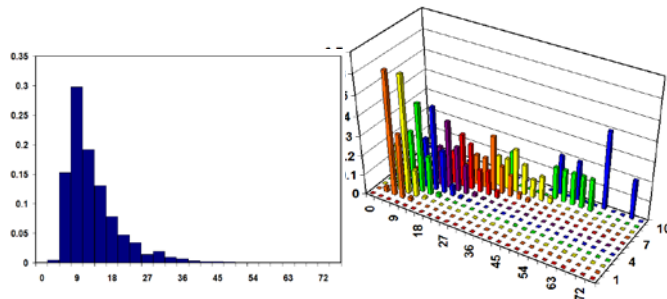
Experimental Data Processing



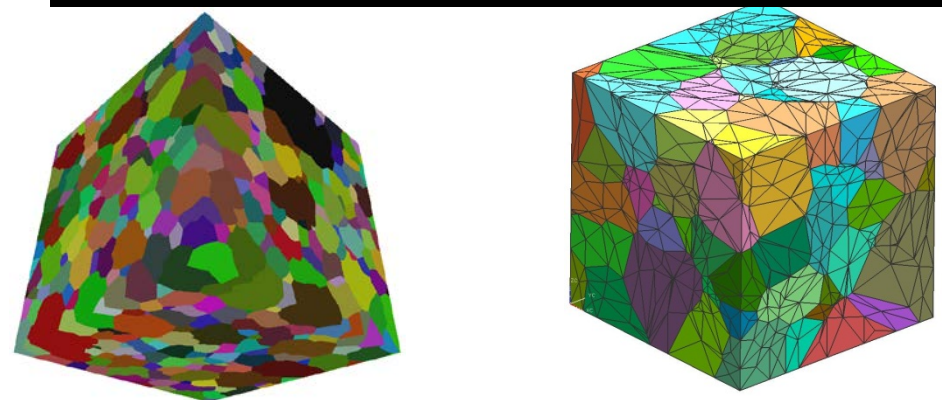
(i) CAD-Based



Distribution and Correlation Functions

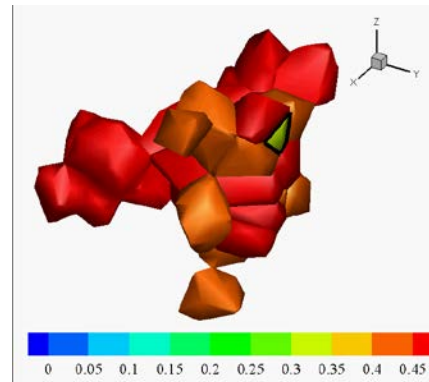


(ii) Statistically Equivalent



Multi-Scale Data Acquisition, Characterization & Image-Based Virtual Models

- High-fidelity 3D characterization provides information at multiple length scales, particularly about “outlier” features which control extreme events.



- Image-based models from the microstructural data. serve as computational microstructural RVE models, e.g. of polycrystalline metals and poly-phase composites.

III. Experimental Methods for Constitutive Models, Response Functions and Failure Processes

- Model calibration and validation over a range of operating conditions.
- Identify underlying mechanisms and provide the models with the requisite fundamental physics, chemistry, and materials science.
- Provide model parameters, validate key predictions, and supplement and extend the range of validity and reliability of the models.

IV. Probabilistic Modeling & Uncertainty Quantification

- **From Deterministic to Stochastic Homogenization**
- Statistically Equivalent RVE (SERVE) use statistical functions to estimate RVE's.
- Statistical Volume Element (SVE) designates a random sample of microstructure that is too small to satisfy the statistical homogeneity requirements. Requires stochastic analysis on each scale
- Stochastic upscaling and stochastic homogenization: stochastic correctors to standard homogenization

Probabilistic Modeling & Uncertainty Quantification

Validation with Experiments at Relevant Scales

- Ensures that the model addresses the right physical problem at each relevant scale as well as interfaces
- Uncertainty Quantification with respect to physical experiments at each scale and interfaces

Summary

Workshop theme is consistent with current trends in ICMSE to guide the design of novel systems that meet specifications of performance and reliability

